

Reflective Boundary conditions in Discontinuous Galerkin Methods for Boltzmann-Poisson Models of Electron Transport in Semiconductors and Zero Flux Condition for General Mixed Reflection

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Abstract

We shall discuss the use of Discontinuous Galerkin (DG) Finite Element Methods to solve Boltzmann - Poisson (BP) models of electron transport in semiconductor devices at nano scales. We consider the mathematical and numerical modeling of Reflective Boundary Conditions in 2D devices and their implementation in DG-BP schemes. We study the specular, diffusive and mixed reflection BC on physical boundaries of the device for the modeling of surface roughness, comparing the influence of these different reflection cases in the computational prediction of moments close to the boundaries and their associated scale. We observe an effect due to diffusivity at the reflection boundaries over the kinetic moments of the probability density function, whose influence is not restricted to the boundaries but rather over the position space domain.

1 Introduction

The dynamics of electronic transport in modern semiconductor devices can be described by the semiclassical Boltzmann-Poisson (BP) model

$$\frac{\partial f_i}{\partial t} + \frac{1}{\hbar} \nabla_{\vec{k}} \varepsilon_i \cdot \nabla_{\vec{x}} f_i - \frac{q_i}{\hbar} \vec{E} \cdot \nabla_{\vec{k}} f_i = \sum_j Q_{i,j} \quad (1.1)$$

$$\nabla_{\vec{x}} \cdot (\epsilon \nabla_{\vec{x}} V) = \sum_i q_i \rho_i - N(\vec{x}), \vec{E} = -\nabla_{\vec{x}} V \quad (1.2)$$

$f_i(\vec{x}, \vec{k}, t)$ is the probability density function (pdf) over phase space (\vec{x}, \vec{k}) of a carrier in the i -th energy band in position \vec{x} , with crystal momentum $\hbar \vec{k}$ at time t . The collision operators $Q_{i,j}(f_i, f_j)$ model i -th and j -th carrier recombinations, collisions with phonons or generation effects. $\vec{E}(\vec{x}, t)$ is the electric field, $\varepsilon_i(\vec{k})$ is the i -th energy band surface, the i -th charge density $\rho_i(t, \vec{x})$ is the k -average of f_i , and $N(\vec{x})$ is the doping profile.

The BP model for electron transport on a single conduction energy band for electrons has the form

$$\frac{\partial f}{\partial t} + \frac{1}{\hbar} \nabla_{\vec{k}} \varepsilon \cdot \nabla_{\vec{x}} f - \frac{q}{\hbar} \vec{E} \cdot \nabla_{\vec{k}} f = Q(f) \quad (1.3)$$

$$\nabla_{\vec{x}} \cdot (\epsilon \nabla_{\vec{x}} V) = q [\rho(\vec{x}, t) - N(\vec{x})], \quad \vec{E} = -\nabla_{\vec{x}} V, \quad (1.4)$$

with the quantum mechanical electron group velocity $\frac{1}{\hbar} \nabla_{\vec{k}} \varepsilon(\vec{k})$, and the electron density $\rho(\vec{x}, t) = \int_{\Omega_{\vec{k}}} f(\vec{x}, \vec{k}, t) d\vec{k}$.

The semi-classical Boltzmann description of electron transport in semiconductors is, for a truly 3-D device, an equation in six dimensions plus time when the device is not in steady state. The heavy computational cost is the main reason why the BP system had been traditionally solved numerically by means of Direct Simulation Monte Carlo (DSMC) methods [11]. However, after the pioneer work [12], in recent years, deterministic solvers to the BP system were proposed in [13, 14, 15, 16, 17, 18, 19]. These methods provide accurate results which, in general, agree well with those obtained from Monte Carlo (DSMC) simulations, often at a fractional computational time. Moreover, these type of solvers can resolve transient details for the electron probability density function f , which are difficult to compute with DSMC simulators.

The initial methods proposed in [15, 16, 17, 18] using weighted essentially non-oscillatory (WENO) finite difference schemes to solve the Boltzmann-Poisson system, had the advantage that the scheme is relatively simple to code and very stable even on coarse meshes for solutions containing sharp gradient regions. However, a disadvantage of the WENO methods is that it requires smooth meshes to achieve high order accuracy, hence it is not very flexible for adaptive meshes.

Motivated by the easy *hp*-adaptivity and the simple communication pattern of the discontinuous Galerkin (DG) methods for macroscopic (fluid level) models [20, 21, 22, 23], it was proposed in [24, 25] to implement a DG solver to the full Boltzmann equation, that is capable of capturing transients of the probability density function.

In the previous work [24, 25], the first DG solver for (1.1)-(2.21) was proposed, and some numerical calculations were shown for one and two-dimensional devices. In [26], the DG-LDG scheme for the Boltzmann-Poisson system was carefully formulated, and extensive numerical studies were performed to validate the calculations. Such scheme models electron transport along the conduction band for 1D diodes and 2D double gate MOSFET devices with an analytic Kane energy band model.

A DG method for full conduction bands BP models was proposed in [27], following the lines of the schemes in [24, 25, 26], generalizing the solver that uses the Kane non-parabolic band and adapting it to treat the full energy band case. A preliminary benchmark of numerical results shows that the direct evaluation of the Dirac delta function can be avoided, and so an accurate high-order

simulation with comparable computational cost to the analytic band cases is possible. It would be more difficult or even unpractical to produce the full band computation with other transport scheme. It is worth to notice that a high-order positivity-preserving DG scheme for linear Vlasov-Boltzmann transport equations, under the action of quadratically confined electrostatic potentials, independent of the electron distribution, has been developed in [28]. The authors there show that these DG schemes conserve mass and preserve the positivity of the solution without sacrificing accuracy. In addition, the standard semi-discrete schemes were studied showing stability and error estimates.

The type of DG method discussed in this paper, as was done in [26], belongs to a class of finite element methods originally devised to solve hyperbolic conservation laws containing only first order spatial derivatives, e.g. [33, 34, 35, 36, 37]. Using a piecewise polynomial space for both the test and trial functions in the spatial variables, and coupled with explicit and nonlinearly stable high order Runge-Kutta time discretization, the DG method is a conservative scheme that has the advantage of flexibility for arbitrarily unstructured meshes, with a compact stencil, and with the ability to easily accommodate arbitrary *hp*-adaptivity. For more details about DG scheme for convection dominated problems, we refer to the review paper [38], later generalized to the Local DG (LDG) method to solve the convection diffusion equations [39] and elliptic equations [40].

Regarding Boundary Conditions (BC), there are several kinds of BC for BP semiconductor models. They vary according to the considered device and physical situation. For example, in the case of electron transport along a single conduction band the following BC could arise:

Charge neutrality boundary conditions, given by [4]

$$f_{out}(t, \vec{x}, \vec{k}) \Big|_{\Gamma} = N_D(\vec{x}) \frac{f_{in}(t, \vec{x}, \vec{k})}{\rho_{in}(t, \vec{x})} \Big|_{\Gamma}, \quad \Gamma \text{ subset of } \partial\Omega_{\vec{x}} \quad (1.5)$$

This BC is imposed in source and drain boundaries where electric currents enter or exit the device in order to obtain there the condition $\rho_{out}(\vec{x}, t) - N_D(\vec{x}) = 0$.

Reflective BC happen in insulating boundaries, usually defined by a Neumann boundary Γ_N , of 2D and 3D devices. In general, Reflective BC can be formulated as the values of the pdf at the inflow boundary being dependent on the outflow boundary values

$$f(\vec{x}, \vec{k}, t) \Big|_{\Gamma_{N-}} = F_R(f|_{\Gamma_{N+}}), \quad (1.6)$$

where the Neumann Inflow Boundary is defined as

$$\Gamma_N^- = \{(\vec{x}, \vec{k}) \mid \vec{x} \in \Gamma_N, \vec{k} \in \Omega_k, \vec{v}(\vec{k}) \cdot \eta(\vec{x}) < 0\}, \quad (1.7)$$

$$\vec{v}(\vec{k}) = \frac{1}{\hbar} \nabla_{\vec{k}} \varepsilon(\vec{k}), \quad (1.8)$$

$\eta(\vec{x})$ outward unit normal. The Neumann Outflow Boundary is defined as

$$\Gamma_N^+ = \{(\vec{x}, \vec{k}) \mid \vec{x} \in \Gamma_N, \vec{k} \in \Omega_k, \vec{v}(\vec{k}) \cdot \eta(\vec{x}) > 0\}. \quad (1.9)$$

Specular Reflection BC over the Neumann Inflow Boundary is imposed by

$$f|_-(\vec{x}, \vec{k}, t) = F_S(f|_+) = f|_+(\vec{x}, \vec{k}', t) \quad \text{for } (\vec{x}, \vec{k}) \in \Gamma_N^-, \quad t > 0, \quad (1.10)$$

$$(\vec{x}, \vec{k}') \in \Gamma_N^+, \quad \vec{k}' \text{ s.t. } \vec{v}(\vec{k}') = \vec{v}(\vec{k}) - 2(\vec{v}(\vec{k}) \cdot \eta(\vec{x}))\eta(\vec{x}). \quad (1.11)$$

Diffusive reflection is a known condition from the kinetic theory for gas dynamics, in which the distribution function at the Inflow boundary is proportional to a Maxwellian [1], [2]

$$f|_-(\vec{x}, \vec{k}, t) = F_D(f|_+) = C \sigma \{f|_+\}(\vec{x}, t) e^{-\varepsilon(\vec{k})/K_B T}, \quad (\vec{x}, \vec{k}) \in \Gamma_N^-, \quad (1.12)$$

$$\sigma \{f|_+\}(\vec{x}, t) = \int_{\vec{v}(\vec{k}) \cdot \eta > 0} \vec{v}(\vec{k}) \cdot \eta(\vec{x}) f|_+(\vec{x}, \vec{k}, t) dk. \quad (1.13)$$

Mixed reflection BC models the reflection of the electrons from a rough boundary, giving the reflected wave a linear convex combination of a specular and a diffuse component, as in the following formula:

$$\begin{aligned} f|_-(\vec{x}, \vec{k}, t) &= F_M(f|_+) = p F_S(f|_+) + (1-p) F_D(f|_+) \\ &= p f|_+(\vec{x}, \vec{k}', t) + (1-p) C \sigma \{f|_+\}(\vec{x}, t) e^{-\frac{\varepsilon(\vec{k})}{K_B T}}, \quad (\vec{x}, \vec{k}) \in \Gamma_N^-. \end{aligned} \quad (1.14)$$

p is sometimes called specularity parameter. It can either be constant or a function of the momentum $p(\vec{k})$. For example, the work by Soffer [5] studies a statistical model for the electrical conduction in metals, and derives a specularity parameter $p(\vec{k})$ which depends on the momentum. It is given by

$$p(\vec{k}) = e^{-4l_r^2 |k|^2 \cos^2 \Theta} \quad (1.15)$$

where l_r is the rms height of rough interface, and Θ_B is the angle between the incident electron and the interface surface normal.

Reflection BC is a widely studied topic in the context of the Kinetic Theory of Gases modelled by Boltzmann - Equations. However, there is few work existent related to the study of the effect of reflection BC, such as diffusive, specular, and mixed reflection, in the context of Boltzmann models for electron transport in semiconductors. A non-exhaustive list of references where reflection BC are studied for Boltzmann Equations in the context of Kinetic Theory of Gases would include the works of Cercignani [3] and Sone [1], where the specular, diffusive, and mixed reflection BC are formulated for the Boltzmann Eq. for gases. V. D. Borman, S. Yu. Krylov, A. V. Chayanov [6] study the nonequilibrium phenomena at a gas-solid interface. The paper of Brull, Charrier, Mieussens [7] studies the gas-surface interaction at a nano-scale and the boundary conditions for the associated Boltzmann equation. Struchtrup [8] studies as well the Maxwell boundary condition and velocity dependent accommodation coefficients in the context of gases mentioned. In the context of the physics of

electron transport, Soffer [5] studies a statistical model for the electrical conduction in metals, and derives under certain assumptions, analytical formulas for the specular parameter $p(\vec{k})$ associated to this physical phenomena, which we mentioned above in (1.15). In the case of semiconductors, the reference book of Markowich, Ringhofer, & Schmeiser [9] discusses the mathematical definition of boundaries according to the physics of semiconductors, and according to the kind of BC to be imposed at those boundaries: Dirichlet, Neumann, Inflow and Outflow boundaries. A work of particular importance for our paper is the one by Cercignani, Gamba, and Levermore [4]. They study high field approximations to a Boltzmann-Poisson system and boundary conditions in a semiconductor. The BP system for electrons in a semiconductor in the case of high fields and small devices is considered. Boundary conditions are proposed at the kinetic level that yield charge neutrality at ohmic contacts, which are Dirichlet boundaries, and at insulating Neumann boundaries. Both BC, either the one yielding charge neutrality at Dirichlet boundaries, or the one rendering zero flux of electrons at the boundary, assume that the pdf is proportional to a ground state associated to an asymptotic expansion of a dimensionless Boltzmann-Poisson system. Then they study closures of moment equations and BC for both the pdf and for the moment closures. Jüngel mentions in his semiconductors book [2] the different kinds of reflection BC common on the kinetic theory of gases, specular, diffusive, and mixed reflection but no further study of these reflection BC in the context of semiconductors is pursued.

We intend to present in this paper a mathematical, numerical, and computational study of the effect of diffusive, specular, and mixed reflection BC in Boltzmann-Poisson models of electron transport in semiconductors, solved by means of Discontinuous Galerkin FEM solvers. We study the mathematical formulation of these reflection BC in the context of BP models for semiconductors, and derive equivalent numerical formulations of the diffusive and mixed reflection BC with non-constant $p(\vec{k})$, such that an equivalent numerical zero flux condition is satisfied pointwise at the insulating Neumann boundaries at the numerical level. We present preliminary numerical simulations for a 2D bulk silicon diode with an applied bias and reflective BC, comparing the effects of specular, diffusive, and mixed reflection in the simulations.

2 BP system with \vec{k} coordinate transformation assuming a Kane Energy Band

The Kane Energy Band Model is a dispersion relation between the conduction energy band ε (measured from a local minimum) and the norm of the electron wave vector $|k|$, given by the analytical function (α is a constant parameter, m^* is the electron reduced mass for Si, and \hbar is Planck's constant):

$$\varepsilon(1 + \alpha\varepsilon) = \frac{\hbar^2 |k|^2}{2m^*} \quad (2.16)$$

For our preliminary numerical studies we will use a Boltzmann-Poisson model as in [26], in which the conduction energy band is assumed to be given by a Kane model. We use the following dimensionalized variables, with the related characteristic parameters:

$$t = t/t_*, (x, y) = \vec{x}/\ell_*, \ell_* = 10^{-6}m, t_* = 10^{-12}s, V_* = 1V$$

A transformed Boltzmann transport equation is used as in [26] as well, where the coordinates used to describe \vec{k} are: μ , the cosine of the polar angle, the azimuthal angle φ , and the dimensionless Kane Energy $w = \varepsilon/K_B T$, which is assumed as the conduction energy band (K_B is Boltzmann's constant, T is the lattice temperature, and $\alpha_K = \alpha K_B T$). So:

$$\vec{k}(w, \mu, \varphi) = \frac{\sqrt{2m^*k_B T_L}}{\hbar} \sqrt{w(1 + \alpha_K w)} \left(\mu, \sqrt{1 - \mu^2} \cos \varphi, \sqrt{1 - \mu^2} \sin \varphi \right) \quad (2.17)$$

A new unknown function Φ is used in the transformed Boltzmann Eq. [26], which is proportional to the Jacobian of the transformation and to the density of states (up to a constant factor):

$$\Phi(t, x, y, w, \mu, \varphi) = s(w) f(t, \vec{x}, \vec{k}),$$

where

$$s(w) = \sqrt{w(1 + \alpha_K w)} (1 + 2\alpha_K w) \quad (2.18)$$

The transformed Boltzmann transport equation for Φ used in [26] is:

$$\frac{\partial \Phi}{\partial t} + \frac{\partial}{\partial x}(g_1 \Phi) + \frac{\partial}{\partial y}(g_2 \Phi) + \frac{\partial}{\partial w}(g_3 \Phi) + \frac{\partial}{\partial \mu}(g_4 \Phi) + \frac{\partial}{\partial \varphi}(g_5 \Phi) = C(\Phi) \quad (2.19)$$

(g_1, g_2) represent the 2D cartesian components of the electron velocity $\frac{1}{\hbar} \nabla_{\vec{k}} \varepsilon(\vec{k})$, in the coordinate system (w, μ, φ) .

(g_3, g_4, g_5) represent the transport in the phase space of the new momentum coordinates (w, μ, φ) due to the self consistent electric field

$$\vec{E}(t, x, y) = (E_x(t, x, y), E_y(t, x, y), 0)$$

$$\begin{aligned}
g_1(\cdot) &= c_x \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} \mu, \\
g_2(\cdot) &= c_x \frac{\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} \sqrt{1-\mu^2} \cos \varphi, \\
g_3(\cdot) &= -c_k \frac{2\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} \left[\mu E_x(t, x, y) + \sqrt{1-\mu^2} \cos \varphi E_y(t, x, y) \right], \\
&= -c_k \frac{2\sqrt{w(1+\alpha_K w)}}{1+2\alpha_K w} \hat{e}_w \cdot \vec{E}(t, x, y), \\
g_4(\cdot) &= -c_k \frac{\sqrt{1-\mu^2}}{\sqrt{w(1+\alpha_K w)}} \left[\sqrt{1-\mu^2} E_x(t, x, y) - \mu \cos \varphi E_y(t, x, y) \right], \\
&= -c_k \frac{\sqrt{1-\mu^2}}{\sqrt{w(1+\alpha_K w)}} \hat{e}_\mu \cdot \vec{E}(t, x, y), \\
g_5(\cdot) &= -c_k \frac{-\sin \varphi}{\sqrt{w(1+\alpha_K w)} \sqrt{1-\mu^2}} E_y(t, x, y) \\
&= -c_k \frac{1}{\sqrt{w(1+\alpha_K w)} \sqrt{1-\mu^2}} \hat{e}_\varphi \cdot \vec{E}(t, x, y),
\end{aligned}$$

with

$$c_x = \frac{t_*}{\ell_*} \sqrt{\frac{2k_B T_L}{m^*}} \quad \text{and} \quad c_k = \frac{t_* q E_*}{\sqrt{2m^* k_B T_L}}.$$

and $\hat{e}_w, \hat{e}_\mu, \hat{e}_\varphi$ the orthonormal vector basis in our momentum coordinate space.

The right hand side of (2.19) is the collision operator (having applied the Dirac Delta's due to electron-phonon scattering, which depend on the energy differences between transitions)

$$\begin{aligned}
C(\Phi)(t, x, y, w, \mu, \varphi) &= s(w) \left\{ c_0 \int_0^\pi d\varphi' \int_{-1}^1 d\mu' \Phi(t, x, y, w, \mu', \varphi') \right. \\
&+ \left. \int_0^\pi d\varphi' \int_{-1}^1 d\mu' [c_+ \Phi(t, x, y, w + \gamma, \mu', \varphi') + c_- \Phi(t, x, y, w - \gamma, \mu', \varphi')] \right\} \\
&- \Phi(t, x, y, w, \mu, \varphi) 2\pi [c_0 s(w) + c_+ s(w - \gamma) + c_- s(w + \gamma)],
\end{aligned}$$

with the dimensionless parameters

$$(c_0, c_+, c_-) = \frac{2m^* t_*}{\hbar^3} \sqrt{2m^* k_B T_L} (K_0, (n_q + 1)K, n_q K), \quad \gamma = \frac{\hbar \omega_p}{k_B T_L}$$

The electron density is:

$$n(t_*, \ell_* x, \ell_* y) = \int_{\mathbb{R}^3} f(t_*, \ell_* x, \ell_* y, \mathbf{k}) d\mathbf{k} = \left(\frac{\sqrt{2m^* k_B T_L}}{\hbar} \right)^3 \rho(t, x, y),$$

where

$$\rho(t, x, y) = \int_0^{+\infty} dw \int_{-1}^1 d\mu \int_0^\pi d\varphi \Phi(t, x, y, w, \mu, \varphi). \quad (2.20)$$

Hence, the dimensionless Poisson equation is

$$\frac{\partial}{\partial x} \left(\epsilon_r \frac{\partial \Psi}{\partial x} \right) + \frac{\partial}{\partial y} \left(\epsilon_r \frac{\partial \Psi}{\partial y} \right) = c_p [\rho(t, x, y) - \mathcal{N}_D(x, y)] \quad (2.21)$$

with

$$\mathcal{N}_D(x, y) = \left(\frac{\sqrt{2m^*k_B T_L}}{\hbar} \right)^{-3} N_D(\ell_* x, \ell_* y) \text{ and } c_p = \left(\frac{\sqrt{2m^*k_B T_L}}{\hbar} \right)^3 \frac{\ell_*^2 q}{\epsilon_0}.$$

3 Discontinuous Galerkin Method for Transformed Boltzmann - Poisson System and Implementation of Boundary Conditions

The domain of the devices to be considered can be represented by means of a rectangular grid in both position and momentum space. This rectangular grid, bidimensional in position space and tridimensional in momentum space, is defined in the following way:

$$\Omega_{ijkmn} = \underbrace{\left[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}} \right] \times \left[y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}} \right]}_{X_{ij}} \times \underbrace{\left[w_{k-\frac{1}{2}}, w_{k+\frac{1}{2}} \right] \times \left[\mu_{m-\frac{1}{2}}, \mu_{m+\frac{1}{2}} \right] \times \left[\varphi_{n-\frac{1}{2}}, \varphi_{n+\frac{1}{2}} \right]}_{K_{kmn}}$$

where $i = 1, \dots, N_x$, $j = 1, \dots, N_y$, $k = 1, \dots, N_w$, $m = 1, \dots, N_\mu$, $n = 1, \dots, N_\varphi$,

$$x_{i \pm \frac{1}{2}} = x_i \pm \frac{\Delta x_i}{2}, \quad y_{j \pm \frac{1}{2}} = y_j \pm \frac{\Delta y_j}{2},$$

$$w_{k \pm \frac{1}{2}} = w_k \pm \frac{\Delta w_k}{2}, \quad \mu_{m \pm \frac{1}{2}} = \mu_m \pm \frac{\Delta \mu_m}{2}, \quad \varphi_{n \pm \frac{1}{2}} = \varphi_n \pm \frac{\Delta \varphi_n}{2}.$$

The finite dimensional space used to approximate the functions is the space of piecewise continuous polynomials which are piecewise linear in (x, y) and piecewise constant in (w, μ, φ)

$$V_h = \{v : v|_{\Omega_{ijkmn}} \in Q^{1,0}(\Omega_{ijkmn}) = P^1(X_{ij}) \otimes P^0(K_{kmn})\}. \quad (3.22)$$

$Q^{1,0}(\Omega_{ijkmn})$ is the set of tensor product polynomials, linear over the element

$$X_{ij} = \left[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}} \right] \times \left[y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}} \right] \text{ and constant over the element } K_{kmn} = \left[w_{k-\frac{1}{2}}, w_{k+\frac{1}{2}} \right] \times \left[\mu_{m-\frac{1}{2}}, \mu_{m+\frac{1}{2}} \right] \times \left[\varphi_{n-\frac{1}{2}}, \varphi_{n+\frac{1}{2}} \right].$$

Φ_h will denote the piecewise polynomial approximation of Φ over elements Ω_I ,

$$\Phi_h = \sum_I \chi_I(x, y, w, \mu, \varphi) \left[T_I(t) + X_I(t) \frac{(x - x_i)}{\Delta x_i/2} + Y_I(t) \frac{(y - y_j)}{\Delta y_j/2} \right], \quad I = (i, j, k, m, n).$$

Under this approximation, the density on the cell $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}] \times [y_{j-\frac{1}{2}}, y_{j+\frac{1}{2}}]$ is

$$\begin{aligned}
\rho_h(t, x, y) &= \sum_{k=1}^{N_w} \sum_{m=1}^{N_\mu} \sum_{n=1}^{N_\varphi} \left[T_{ijkmn} + X_{ijkmn} \frac{(x - x_i)}{\Delta x_i/2} + Y_{ijkmn} \frac{(y - y_j)}{\Delta y_j/2} \right] \Delta w_k \Delta \mu_m \Delta \varphi_n \\
&= \sum_{k=1}^{N_w} \sum_{m=1}^{N_\mu} \sum_{n=1}^{N_\varphi} T_{ijkmn} \Delta w_k \Delta \mu_m \Delta \varphi_n \\
&\quad + \left(\sum_{k=1}^{N_w} \sum_{m=1}^{N_\mu} \sum_{n=1}^{N_\varphi} X_{ijkmn} \Delta w_k \Delta \mu_m \Delta \varphi_n \right) \frac{(x - x_i)}{\Delta x_i/2} \\
&\quad + \left(\sum_{k=1}^{N_w} \sum_{m=1}^{N_\mu} \sum_{n=1}^{N_\varphi} Y_{ijkmn} \Delta w_k \Delta \mu_m \Delta \varphi_n \right) \frac{(y - y_j)}{\Delta y_j/2}
\end{aligned}$$

3.1 DG Formulation for Transformed Boltzmann Eq.

The Discontinuous Galerkin formulation for the Boltzmann equation (2.19) is:

Find $\Phi_h \in V_h$, s.t.

$$\begin{aligned}
&\int_{\Omega_{ijkmn}} (\Phi_h)_t v_h d\Omega - \int_{\Omega_{ijkmn}} g_1 \Phi_h (v_h)_x d\Omega - \int_{\Omega_{ijkmn}} g_2 \Phi_h (v_h)_y d\Omega \\
&\quad + F_x^+ - F_x^- + F_y^+ - F_y^- + F_w^+ - F_w^- + F_\mu^+ - F_\mu^- + F_\varphi^+ - F_\varphi^- = \int_{\Omega_{ijkmn}} C(\Phi_h) v_h d\Omega.
\end{aligned} \tag{3.23}$$

for any test function $v_h \in V_h$. In (3.23), the boundary integrals are given by:

$$F_x^\pm = \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \int_{w_{k-\frac{1}{2}}}^{w_{k+\frac{1}{2}}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} \widehat{g_1 \Phi} v_h^\mp(x_{i\pm\frac{1}{2}}, y, w, \mu, \varphi) dy dw d\mu d\varphi,$$

$$F_y^\pm = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{w_{k-\frac{1}{2}}}^{w_{k+\frac{1}{2}}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} \widehat{g_2 \Phi} v_h^\mp(x, y_{j\pm\frac{1}{2}}, w, \mu, \varphi) dx dw d\mu d\varphi,$$

$$F_w^\pm = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} \widehat{g_3 \Phi} v_h^\mp(x, y, w_{k\pm\frac{1}{2}}, \mu, \varphi) dx dy d\mu d\varphi,$$

$$F_\mu^\pm = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \int_{w_{k-\frac{1}{2}}}^{w_{k+\frac{1}{2}}} \int_{\varphi_{n-\frac{1}{2}}}^{\varphi_{n+\frac{1}{2}}} \widehat{g_4 \Phi} v_h^\mp(x, y, w, \mu_{m\pm\frac{1}{2}}, \varphi) dx dy dw d\varphi,$$

$$F_\varphi^\pm = \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \int_{y_{j-\frac{1}{2}}}^{y_{j+\frac{1}{2}}} \int_{w_{k-\frac{1}{2}}}^{w_{k+\frac{1}{2}}} \int_{\mu_{m-\frac{1}{2}}}^{\mu_{m+\frac{1}{2}}} \widehat{g_5 \Phi} v_h^\mp(x, y, w, \mu, \varphi_{n\pm\frac{1}{2}}) dx dy dw d\mu,$$

where the upwind numerical fluxes $\widehat{g_s \Phi}$, $s = 1, \dots, 5$ are defined as

$$\begin{aligned}
\widehat{g_1\Phi}|_{x_{i\pm 1/2}} &= \left(\frac{g_1 + |g_1|}{2}\right) \Phi_h|_{x_{i\pm 1/2}}^- + \left(\frac{g_1 - |g_1|}{2}\right) \Phi_h|_{x_{i\pm 1/2}}^+ \\
\widehat{g_2\Phi}|_{y_{j\pm 1/2}} &= \left(\frac{g_2 + |g_2|}{2}\right) \Phi_h|_{y_{j\pm 1/2}}^- + \left(\frac{g_2 - |g_2|}{2}\right) \Phi_h|_{y_{j\pm 1/2}}^+ \\
\widehat{g_3\Phi}|_{w_{k\pm 1/2}} &= \left(\frac{g_3 + |g_3|}{2}\right) \Phi_h|_{w_{k\pm 1/2}}^- + \left(\frac{g_3 - |g_3|}{2}\right) \Phi_h|_{w_{k\pm 1/2}}^+ \\
\widehat{g_4\Phi}|_{\mu_{m\pm 1/2}} &= \left(\frac{g_4 + |g_4|}{2}\right) \Phi_h|_{\mu_{m\pm 1/2}}^- + \left(\frac{g_4 - |g_4|}{2}\right) \Phi_h|_{\mu_{m\pm 1/2}}^+ \\
\widehat{g_5\Phi}|_{\varphi_{n\pm 1/2}} &= \left(\frac{g_5 + |g_5|}{2}\right) \Phi_h|_{\varphi_{n\pm 1/2}}^- + \left(\frac{g_5 - |g_5|}{2}\right) \Phi_h|_{\varphi_{n\pm 1/2}}^+ \quad (3.24)
\end{aligned}$$

The Poisson equation (2.21) is solved by the LDG method as in [26]. By means of this scheme we find a solution $\Psi_h, q_h, s_h \in W_h^1$, where $(q, s) = (\partial_x \Psi, \partial_y \Psi)$ and $W_h^1 = \{v : v|_{X_{ij}} \in P^1(X_{ij})\}$, $P^1(X_{ij})$ the set of linear polynomials on X_{ij} .

3.2 RK-DG Algorithm for BP, from t^n to t^{n+1}

The following RK-DG algorithm for BP is a dynamic extension of the Gummel iteration map. To evolve from time t^n to time t^{n+1} :

- 1.- Compute the electron density $\rho_h(x, y, t)$.
- 2.- Solve Poisson Eq. for the given $\rho_h(x, y, t)$ by Local DG, obtaining the potential Ψ_h and the electric field $\mathbf{E}_h = -(q_h, s_h)$. Compute then the respective transport terms g_s , $s = 1, \dots, 5$.
- 3.- Solve by DG the advection and collision part of the Boltzmann Equation. A Method of Lines (an ODE system) for the time dependent coefficients of Φ_h (degrees of freedom) is obtained.
- 4.-Evolve ODE system by Runge-Kutta from t^n to t^{n+1} .
(If partial time step necessary, repeat Step 1 to 3 as needed).

4 Boundary Conditions Implementation for 2D- \vec{x} , 3D- \vec{k} devices at x, w, μ, φ Boundaries

We will consider in this work 2D devices in position space, which need a 3D momentum description for kinetic equations modeling semiconductors. For example, a common device of interest is a 2D double gate MOSFET. A schematic plot of it is given in Figure 4.1. The shadowed region denotes the oxide-silicon region, whereas the rest is the silicon region. Potential bias are applied at the source, drain, and gates. The problem is symmetric about the x-axis.

Another possible 2D problem is the case of a bi-dimensional bulk silicon diode, for which the doping is constant all over the physical domain, and which would have just an applied potential (bias) between the source $x = 0$ and the drain $x = L_x$ (no gates), with insulating reflecting boundaries at $y = 0$ and $y = L_y$.

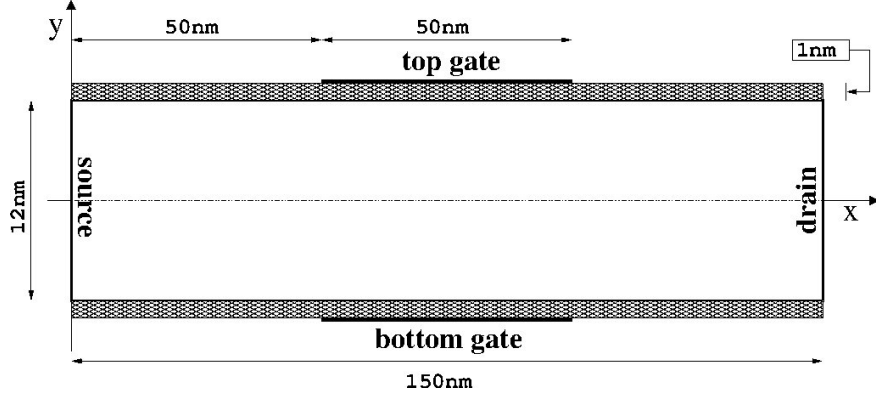


Figure 4.1: Schematic representation of a 2D double gate MOSFET device

We consider in the following sections the different kinds of boundary conditions for 2D devices and their numerical implementation, either at \vec{x} -boundaries or at \vec{w} -boundaries.

4.1 Poisson Eq. Boundary Condition

The BC for Poisson Eq. are imposed over the (x, y) -domain.

For example, for the case of a 2D Double gated MOSFET, Dirichlet BC would be imposed to the potential Ψ , as we have three different applied potentials biases:

$\Psi = 0.5235$ Volts at the source $x = 0$, $\Psi = 1.5235$ Volts at the drain $x = L_x$, $\Psi = 1.06$ Volts at the gates. Homogeneous Neumann BC would be imposed for the rest of the boundaries, that is, $\partial_{\vec{n}} \Psi = 0$.

For the case of a 2D bulk silicon diode, we impose Dirichlet BC for the difference of potential Ψ between source and drain:

$\Psi = 0.5235$ Volts at the source $x = 0$, $\Psi = 1.5235$ Volts at the drain $x = L_x$.

For the boundaries $y = 0, L_y$ we impose Homogeneous Neumann BC too, that is, $\partial_y \Psi|_{y_0} = 0, y_0 = 0, L_y$.

4.2 Charge Neutrality BC

As in [26], at the source and drain contacts, we implement the charge neutrality boundary condition (1.5). Ghost cells for $i = 0$ and $i = N_x + 1$ at the respective boundaries are used, implementing this BC numerically as below:

$$\Phi(i = 0) = \Phi(i = 1) \frac{N_D(i = 1)}{\rho(i = 1)},$$

and

$$\Phi(i = N_x + 1) = \Phi(i = N_x) \frac{N_D(i = N_x)}{\rho(i = N_x)}.$$

4.3 Cut - Off BC

In the (w, μ, φ) -space, we only need to apply a cut-off Boundary Condition. At $w = w_{\max}$, Φ_h is made machine zero:

$$\Phi_h(x, y, w, \mu, \varphi, t)|_{w=w_{\max}} = 0. \quad (4.25)$$

No other boundary condition is necessary for \vec{w} -boundaries, since analytically we have that:

- at $w = 0$, $g_3 = 0$.
- at $\mu = \pm 1$, $g_4 = 0$;
- at $\varphi = 0, \pi$, $g_5 = 0$,

so, at those boundaries, the numerical flux always vanishes.

5 Reflection BC on BP

Reflection Boundary Conditions can be expressed in the following form:

$$f(\vec{x}, \vec{k}, t)|_{\Gamma_{N-}} = F_R(f|_{\Gamma_{N+}}) \quad (5.26)$$

such that the following pointwise zero flux condition is satisfied at reflecting boundaries:

$$\begin{aligned} 0 &= \eta(\vec{x}) \cdot J(\vec{x}, t) = \eta(\vec{x}) \cdot \int_{\Omega_{\vec{k}}} \vec{v}(\vec{k}) f(\vec{x}, \vec{k}, t) d\vec{k} \\ 0 &= \int_{\eta(\vec{x}) \cdot \vec{v}(\vec{k}) > 0} \eta(\vec{x}) \cdot \vec{v}(\vec{k}) f(\vec{x}, \vec{k}, t)|_{\Gamma_{N+}} d\vec{k} + \int_{\eta(\vec{x}) \cdot \vec{v}(\vec{k}) < 0} \eta(\vec{x}) \cdot \vec{v}(\vec{k}) f(\vec{x}, \vec{k}, t)|_{\Gamma_{N-}} d\vec{k} \\ 0 &= \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta f|_{\Gamma_{N+}} d\vec{k} + \int_{\vec{v} \cdot \eta < 0} \vec{v} \cdot \eta F_R(f|_{\Gamma_{N+}}) d\vec{k}, \end{aligned} \quad (5.27)$$

as in the paper [4] of Cercignani, Gamba, and Levermore, where the given BC at Neumann boundaries at the kinetic level is such that the particle flow vanishes at these insulating boundaries.

For simplicity we write $\vec{v} = \vec{v}(\vec{k}) = \nabla_{\vec{k}} \varepsilon(\vec{k}) / \hbar$. We will study three kinds of reflective boundary conditions: specular, diffusive, and mixed reflection. The last one is a convex combination of the previous two, but the convexity parameter can be either constant or momentum dependant, $p(\vec{k})$. We go over the math and numerics related to these conditions below.

5.1 Specular Reflection

It is clear that, at the analytical level, the specular reflection BC (1.10) satisfies the zero flux condition pointwise at reflecting boundaries, since

$$\int_{\eta \cdot \vec{v} > 0} |\eta(\vec{x}) \cdot \vec{v}(\vec{k})| f(\vec{x}, \vec{k}, t)|_{\Gamma_{N^+}} d\vec{k} - \int_{\eta \cdot \vec{v} < 0} |\eta(\vec{x}) \cdot \vec{v}(\vec{k})| f(\vec{x}, \vec{k}', t)|_{\Gamma_{N^+}} d\vec{k} = 0 \quad (5.28)$$

Specular reflection BC in our transformed Boltzmann Eq. for the new coordinate system is mathematically formulated in our problem as

$$\Phi|_-(x, y, w, \mu, \varphi, t) = \Phi|_+(x, y, w, \mu, \pi - \varphi, t), \quad (x, y, w, \mu, \varphi) \in \Gamma_N^-. \quad (5.29)$$

To impose numerically specular reflection BC at $y = 0, L_y$ in the DG method, we follow the procedure of [26]. We relate the inflow values of the pdf, associated to the outer ghost cells, to the outflow values of the pdf, which are associated to the interior cells adjacent to the boundary, as given below

$$\begin{aligned} \Phi_h|_-(x, y_{1/2}, w, \mu, \varphi, t) &= \Phi_h|_+(x, y_{1/2}, w, \mu, \pi - \varphi, t), \quad y_{1/2} = 0. \\ \Phi_h|_-(x, y_{N_y + \frac{1}{2}}, w, \mu, \varphi, t) &= \Phi_h|_+(x, y_{N_y + \frac{1}{2}}, w, \mu, \pi - \varphi, t), \quad y_{N_y + \frac{1}{2}} = L_y. \end{aligned} \quad (5.30)$$

In the case of the boundary $y_{1/2} = 0$, assuming $\Delta y_0 = \Delta y_1$, $\Delta \varphi_{n'} = \Delta \varphi_n$, with $n' = N_\varphi - n + 1$, if $(x, y_{1/2} - y, w, \mu, \varphi) \in \Omega_{i0kmn}$ then $(x, y_{1/2} + y, w, \mu, \pi - \varphi) \in \Omega_{i1kmn'}$. The values of $\Phi_h|_{y_{1/2}}^\pm$ at the related inner and outer boundary cells Ω_{i0kmn} ($j = 0$) and $\Omega_{i1kmn'}$ ($j = 1$) must be equal at the boundary $y_{1/2} = 0$:

$$\begin{aligned} \Phi_h|_{\Omega_{i0kmn}}^-(x, y_{1/2}, w, \mu, \varphi, t) &= \Phi_h|_{\Omega_{i1kmn'}}^+(x, y_{1/2}, w, \mu, \pi - \varphi, t) \implies \\ T_{i0kmn} + X_{i0kmn} \frac{(x - x_i)}{\Delta x_i/2} + Y_{i0kmn} \frac{(y_{1/2} - y_0)}{\Delta y_0/2} &= \\ T_{i1kmn'} + X_{i1kmn'} \frac{(x - x_i)}{\Delta x_i/2} + Y_{i1kmn'} \frac{(y_{1/2} - y_1)}{\Delta y_1/2}. \end{aligned}$$

Therefore, from the equality above we find the relation between the coefficients of Φ_h at inner and outer adjacent boundary cells, given by

$$T_{i0kmn} = T_{i1kmn'}, \quad X_{i0kmn} = X_{i1kmn'}, \quad Y_{i0kmn} = -Y_{i1kmn'} \quad (5.31)$$

Following an analogous procedure for the boundary $y_{N_y+1/2}$, we have that

$$\begin{aligned} \Phi_h|_{\Omega_{i,N_y+1,kmn}}^-(x, y_{N_y+\frac{1}{2}}, w, \mu, \varphi, t) &= \Phi_h|_{\Omega_{i,N_y,kmn'}}^+(x, y_{N_y+\frac{1}{2}}, w, \mu, \pi - \varphi, t) \implies \\ T_{i,N_y+1,kmn} + X_{i,N_y+1,kmn} \frac{(x - x_i)}{\Delta x_i/2} + Y_{i,N_y+1,kmn} \frac{(y_{N_y+\frac{1}{2}} - y_{N_y+1})}{\Delta y_{N_y+1}/2} &= \\ T_{i,N_y,kmn'} + X_{i,N_y,kmn'} \frac{(x - x_i)}{\Delta x_i/2} + Y_{i,N_y,kmn'} \frac{(y_{N_y+\frac{1}{2}} - y_{N_y})}{\Delta y_{N_y}/2} &\implies \end{aligned} \quad (5.32)$$

$$T_{i,N_y+1,kmn} = T_{i,N_y,kmn'}, \quad X_{i,N_y+1,kmn} = X_{i,N_y,kmn'}, \quad Y_{i,N_y+1,kmn} = -Y_{i,N_y,kmn'}.$$

5.2 Diffusive Reflection

The diffusive reflection BC can be formulated in the following way:

$$f(\vec{x}, \vec{k}, t)|_- = F_D(f|_+) = C \sigma \{f|_+\}(\vec{x}, t) e^{-\varepsilon(\vec{k})/K_B T_L}, \quad (\vec{x}, \vec{k}) \in \Gamma_N^-, \quad (5.33)$$

where $\sigma \{f|_+\}(\vec{x}, t) = \sigma(\vec{x}, t)$ and $C = C\{\eta(\vec{x})\}$ are the function and parameter such that the zero flux condition is satisfied at each of the points of the Neumann Boundary:

$$\begin{aligned} 0 &= \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta f|_{\Gamma_{N+}} d\vec{k} + \int_{\vec{v} \cdot \eta < 0} \vec{v} \cdot \eta \left[C \sigma(\vec{x}, t) e^{-\varepsilon(\vec{k})/K_B T_L} \right] d\vec{k}, \\ 0 &= \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta f|_{\Gamma_{N+}} d\vec{k} - \sigma(\vec{x}, t) \cdot C \int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| e^{-\varepsilon(\vec{k})/K_B T_L} d\vec{k}. \end{aligned}$$

It follows then that

$$\sigma \{f|_+\}(\vec{x}, t) = \int_{\vec{v}(\vec{k}) \cdot \eta > 0} \vec{v} \cdot \eta f|_{\Gamma_{N+}}(\vec{x}, \vec{k}, t) d\vec{k}, \quad (5.34)$$

$$C \{\eta(\vec{x})\} = \left(\int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| e^{-\varepsilon(\vec{k})/K_B T_L} d\vec{k} \right)^{-1}, \quad (5.35)$$

$$f(\vec{x}, \vec{k}, t)|_- = \frac{e^{-\varepsilon(\vec{k})/K_B T_L} \int_{\vec{v}(\vec{k}) \cdot \eta > 0} \vec{v} \cdot \eta f|_{\Gamma_{N+}}(\vec{x}, \vec{k}, t) d\vec{k}}{\int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| e^{-\varepsilon(\vec{k})/K_B T_L} d\vec{k}}. \quad (5.36)$$

The diffusive reflection BC, formulated in terms of the unknown function Φ of the transformed Boltzmann Equation 2.19, is expressed as

$$\Phi|_-(x, y, w, \mu, \varphi, t) = F_D(\Phi|_+) = C \sigma \{\Phi|_+\}(x, y, t) e^{-w} s(w), \quad (5.37)$$

$$\sigma(x, y, t) = \int_{(g_1, g_2) \cdot \eta > 0} \eta \cdot (g_1, g_2)(w, \mu, \varphi) \Phi|_+ dw d\mu d\varphi \quad (5.38)$$

$$C(\eta) = \left(\int_{(g_1, g_2) \cdot \eta < 0} |(g_1, g_2) \cdot \eta| e^{-w} s(w) dw d\mu d\varphi \right)^{-1} \quad (5.39)$$

We have, over the portion of the boundary considered, that $\eta = (0, -1, 0)$ for $y = 0$ and $\eta = (0, 1, 0)$ for $y = L_y$. Therefore:

$$\Phi|_-(x, y_b, w, t) = \frac{e^{-w} s(w) \int_{-g_2 > 0} |g_2| \Phi|_+ dw d\mu d\varphi}{\int_{-g_2 < 0} |g_2| e^{-w} s(w) dw d\mu d\varphi}, \quad y_b = 0, \quad (5.40)$$

$$\Phi|_-(x, y_b, w, t) = \frac{e^{-w} s(w) \int_{+g_2 > 0} |g_2| \Phi|_+ dw d\mu d\varphi}{\int_{+g_2 < 0} |g_2| e^{-w} s(w) dw d\mu d\varphi}, \quad y_b = L_y. \quad (5.41)$$

5.2.1 Numerical Formulation of Diffusive BC for DG

For the case of the DG numerical method, we have to project the BC to be imposed in the space V_h . Our goal is to have at the numerical level an equivalent pointwise zero flux condition at the reflection boundaries.

We formulate then the diffusive BC for the DG method in the following way:

$$\begin{aligned}\Phi_h|_-(x, y_b, w, \mu, \varphi, t) &= \Pi_h \{F_D(\Phi_h|_+)\} \\ &= \Pi_h \{C \sigma_h \{\Phi_h|_+\} (x, y_b, t) e^{-w} s(w)\}, \quad y_b = 0, L_y.\end{aligned}$$

where $\sigma_h \in V_h$ is a function in our piecewise polynomial space for (x, y) and C is a parameter such that the zero flux condition is satisfied numerically

$$\begin{aligned}0 &= \int_{\vec{g} \cdot \eta > 0} \vec{g} \cdot \eta \Phi_h|_+ d\vec{w} + \int_{\vec{g} \cdot \eta < 0} \vec{g} \cdot \eta \Phi_h|_- d\vec{w} \\ &= \int_{\vec{g} \cdot \eta > 0} \vec{g} \cdot \eta \Phi_h|_+ d\vec{w} + \int_{\vec{g} \cdot \eta < 0} \vec{g} \cdot \eta \Pi_h \{F_D(\Phi_h|_+)\} d\vec{w} \\ &= \int_{\vec{g} \cdot \eta > 0} \vec{g} \cdot \eta \Phi_h|_+ d\vec{w} + \int_{\vec{g} \cdot \eta < 0} \vec{g} \cdot \eta \Pi_h \{C \sigma_h \{\Phi_h|_+\} (x, y_b, t) e^{-w} s(w)\} d\vec{w}\end{aligned} \quad (5.42)$$

In the space V_h of piecewise continuous polynomials which are tensor products of polynomials of degree p in \vec{x} and of degree q in \vec{w} , the following holds:

$$\begin{aligned}\Pi_h \{f_1(\vec{x}) f_2(\vec{w})\} &= \Pi_h \{f_1(\vec{x})\} \Pi_h \{f_2(\vec{w})\}, \\ V_h &= \{v : v|_{\Omega_{ijkmn}} \in Q^{p,q}(\Omega_{ijkmn}) = P^p(X_{ij}) \otimes P^q(K_{kmn})\}.\end{aligned} \quad (5.43)$$

Therefore, for our particular case we have that

$$\Pi_h \{C \sigma_h(x, y_b, t) e^{-w} s(w)\} = C \sigma_h(x, y_b, t) \Pi_h \{e^{-w} s(w)\} \quad (5.44)$$

so for the numerical zero flux condition pointwise we have that

$$\begin{aligned}0 &= \int_{\vec{g} \cdot \eta > 0} \vec{g} \cdot \eta \Phi_h|_+ d\vec{w} + \int_{\vec{g} \cdot \eta < 0} \vec{g} \cdot \eta C \sigma_h \{\Phi_h|_+\} (x, y_b, t) \Pi_h \{e^{-w} s(w)\} d\vec{w} \\ 0 &= \int_{\vec{g} \cdot \eta > 0} \vec{g} \cdot \eta \Phi_h|_+ d\vec{w} - \sigma_h \{\Phi_h|_+\} (x, y_b, t) C \int_{\vec{g} \cdot \eta < 0} |\vec{g} \cdot \eta| \Pi_h \{e^{-w} s(w)\} d\vec{w}\end{aligned}$$

We observe then that we can obtain a numerical equivalent of the pointwise zero flux condition if we define

$$\begin{aligned}\sigma_h \{\Phi_h|_+\} (x, y_b, t) &= \int_{\pm g_2 = \vec{g} \cdot \eta > 0} \vec{g} \cdot \eta \Phi_h|_+ d\vec{w} = \sigma \{\Phi_h|_+\} (x, y_b, t), \quad y_b = 0, L_y. \\ C \{\eta\} &= C \{\pm \hat{y}\} = \left(\int_{\pm g_2 = \vec{g} \cdot \eta < 0} |\vec{g} \cdot \eta| \Pi_h \{e^{-w} s(w)\} d\vec{w} \right)^{-1}, \quad \eta = \pm \hat{y}.\end{aligned}$$

In our particular case, in which we have chosen our function space as piecewise linear in (x, y) and piecewise constant in (w, μ, φ) , the projection of the

Maxwellian is a piecewise constant approximation representing its average value over each momentum cell, that is

$$\Pi_h \{e^{-w} s(w)\} = \sum_{k,m,n} \chi_{kmn} \frac{\int_{kmn} e^{-w} s(w) dw d\mu d\varphi}{\Delta w_k \Delta \mu_m \Delta \varphi_n} = \sum_{k,m,n} \chi_{kmn} \frac{\int_{w_{k-}}^{w_{k+}} e^{-w} s(w) dw}{\Delta w_k} \quad (5.45)$$

Therefore, for the particular space we have chosen, we have that

$$\begin{aligned} \sigma_h \{\Phi_h|_+\}(x, y_b, t) &= \int_{\pm g_2 > 0} \pm g_2 \Phi_h|_+ d\vec{w} = \sigma \{\Phi_h|_+\}(x, y_b, t), \\ y_b = 0 = y_{1/2} \quad (\eta = -\hat{y}), \quad \text{or} \quad y_b = L_y = y_{N_y+1/2} \quad (\eta = +\hat{y}). \\ C^{-1} &= \sum_{k,m,n}^{\pm g_2 < 0} \frac{1}{\Delta w_k} \int_{w_{k-1/2}}^{w_{k+1/2}} e^{-w} s(w) dw \int_{k,m,n} |g_2| dw d\mu d\varphi, \quad \eta = \pm \hat{y}. \\ \Phi_h|_-(x, y_b, w, \mu, \varphi, t) &= C \sigma_h \{\Phi_h|_+\}(x, y_b, t) \Pi_h \{e^{-w} s(w)\}, \quad y_b = 0, L_y. \\ \Phi_h|_-(x, y_b, w, \mu, \varphi, t) &= \frac{\int_{\pm g_2 > 0} |g_2| \Phi_h|_+ d\vec{w} \times \sum_{k,m,n}^{\pm g_2 < 0} \chi_{k,m,n} \int_k e^{-w} s(w) dw / \Delta w_k}{\sum_{k,m,n}^{\pm g_2 < 0} \int_{kmn} |g_2| dw d\mu d\varphi \int_k e^{-w} s(w) dw / \Delta w_k} \end{aligned} \quad (5.46)$$

We notice that the polynomial approximation σ_h is equal to the analytical function σ operating on the polynomial approximation $\Phi_h|_+$. However, the constant C needed in order to achieve the zero flux condition numerically is not equal to the value of this parameter for the analytical case. C is in this case an approximation of the analytical value using a piecewise constant approximation of the Maxwellian (its average over cells).

$\sigma(x, y, t)$ is a piecewise linear polynomial depending on (x, y) with time dependent coefficients. We have that

$$\Phi_h|_+ \in V_h \implies \sigma_h \{\Phi_h|_+\}(x, y, t) = \int_{\pm \cos \varphi > 0} |g_2| \Phi_h|_+ dw d\mu d\varphi \in V_h$$

$\Phi_h|_+$ is such that, at the boundary $y = y_b$ of the cell Ω_{ijkmn} , is given by

$$\Phi_h|_+(t, x, y, w, \mu, \varphi) = T_{ijkmn}(t) + X_{ijkmn}(t) \frac{2(x - x_i)}{\Delta x_i} + Y_{ijkmn}(t) \frac{2(y - y_j)}{\Delta y_j}$$

We define $I = ijkmn$, so in $\Omega_I = X_{ij} \times K_{kmn}$. We will have then

$$\sigma_h(x, y, t) = \sigma_I^0(t) + \sigma_I^x(t) \frac{(x - x_i)}{\Delta x_i/2} + \sigma_I^y(t) \frac{(y - y_j)}{\Delta y_j/2} \quad (5.47)$$

We summarize the main results of the calculations for σ_h and $\Phi_h|_-$, by showing the ones related to $y = L_y$ (the case $y = 0$ is analogous). For the boundary $y = L_y$, the inner cells associated to outflow have $j = N_y$, adjacent to the boundary, whereas the ghost cells related to inflow have the index $j = N_y + 1$. We compute the integral σ_h below.

$$\begin{aligned}
\sigma_h \{ \Phi_h|_+ \} (x, y, t) &= \int_{\cos \varphi \geq 0} \frac{\sqrt{w(1 + \alpha_K w)}}{1 + 2\alpha_K w} \sqrt{1 - \mu^2} \cos \varphi \Phi_h|_+ dw d\mu d\varphi \\
&= \sum_{k, m, n}^{n \leq N_p/2} \int_{K_{kmn}} \frac{\sqrt{w(1 + \alpha_K w)}}{1 + 2\alpha_K w} \sqrt{1 - \mu^2} \cos \varphi \Phi_h|_+ dw d\mu d\varphi
\end{aligned}$$

Therefore, we have, with $I = (i, j, k, m, n)$, $j = N_y$ below, that

$$\begin{aligned}
\sigma_I^0 &= \sum_{k, m, n}^{n \leq N_\varphi/2} T_{iN_y kmn} \int_{w_{k-1/2}}^{w_{k+1/2}} \frac{\sqrt{w(1 + \alpha_K w)}}{1 + 2\alpha_K w} dw \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} \sqrt{1 - \mu^2} d\mu \int_{\varphi_{n-1/2}}^{\varphi_{n+1/2}} \cos \varphi d\varphi \\
\sigma_I^x &= \sum_{k, m, n}^{n \leq N_\varphi/2} X_{iN_y kmn} \int_{w_{k-1/2}}^{w_{k+1/2}} \frac{\sqrt{w(1 + \alpha_K w)}}{1 + 2\alpha_K w} dw \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} \sqrt{1 - \mu^2} d\mu \int_{\varphi_{n-1/2}}^{\varphi_{n+1/2}} \cos \varphi d\varphi \\
\sigma_I^y &= \sum_{k, m, n}^{n \leq N_\varphi/2} Y_{iN_y kmn} \int_{w_{k-1/2}}^{w_{k+1/2}} \frac{\sqrt{w(1 + \alpha_K w)}}{1 + 2\alpha_K w} dw \int_{\mu_{m-1/2}}^{\mu_{m+1/2}} \sqrt{1 - \mu^2} d\mu \int_{\varphi_{n-1/2}}^{\varphi_{n+1/2}} \cos \varphi d\varphi
\end{aligned} \tag{5.48}$$

Once the coefficients of σ_h have been computed, we use them to obtain the polynomial approximation $\Phi_h|_-$, with $j = N_y + 1$, from (5.46)

$$\Phi_h|_{y=L_y}^- = \sum_i \sum_{k, m, n}^{n \geq N_\varphi/2} \chi_{iN_y kmn} C \left[\sigma_I^0 + \sigma_I^x \frac{(x - x_i)}{\Delta x_i/2} + \sigma_I^y (+1) \right] \frac{\int_k e^{-w} s(w) dw}{\Delta w_k} . \tag{5.49}$$

We have at the same time, by definition, that

$$\Phi_h|_{y=L_y}^- = \sum_{i, k, m, n}^{n \geq N_\varphi/2} \chi_{i, N_y+1, kmn} \left[T_{i, N_y+1, k, m, n} + X_{i, N_y+1, k, m, n} \frac{(x - x_i)}{\Delta x_i/2} + Y_{i, N_y+1, k, m, n} (-1) \right] .$$

Therefore, the coefficients for $\Phi_h|_{y=L_y}^-$ are

$$T_{i, N_y+1, kmn}(t) = C \sigma_{iN_y kmn}^0(t) \frac{\int_k e^{-w} s(w) dw}{\Delta w_k} \tag{5.50}$$

$$X_{i, N_y+1, kmn}(t) = C \sigma_{iN_y kmn}^x(t) \frac{\int_k e^{-w} s(w) dw}{\Delta w_k} \tag{5.51}$$

$$Y_{i, N_y+1, kmn}(t) = (-1) C \sigma_{iN_y kmn}^y(t) \frac{\int_k e^{-w} s(w) dw}{\Delta w_k} , \tag{5.52}$$

keeping in mind that our parameter C is given by the formula below

$$C^{-1} = \sum_{k, m, n}^{n \geq N_p/2} \frac{\int_k e^{-w} s(w) dw}{\Delta w_k} \int_k \frac{\sqrt{w(1 + \alpha_K w)}}{1 + 2\alpha_K w} dw \int_m \sqrt{1 - \mu^2} d\mu \int_n \cos \varphi d\varphi . \tag{5.53}$$

5.3 Mixed Reflection

The mixed reflection condition is a convex combination of the specular and diffusive reflections:

$$f(\vec{x}, \vec{k}, t)|_- = pf|_+(\vec{x}, \vec{k}', t) + (1-p)C\sigma\{f|_+\}(\vec{x}, t)e^{-\varepsilon(\vec{k})/K_B T}, \quad (\vec{x}, \vec{k}) \in \Gamma_N^-$$

p is the Specularity Parameter, $0 \leq p \leq 1$. p can be either constant or $p = p(\vec{k})$, a function of the wave vector momentum.

For p constant, it can be shown easily that the previous formulas obtained for the specular and diffusive BC, in particular the previous formulas for $\sigma C(x)$, works also in this case to obtain a zero flux condition at the Neumann boundaries:

$$\begin{aligned} \eta \cdot J &= \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta f|_{\Gamma_{N^+}} d\vec{k} + \int_{\vec{v} \cdot \eta < 0} \vec{v} \cdot \eta \left[pf(\vec{x}, \vec{k}', t)|_{\Gamma_{N^+}} + (1-p)Ce^{-\varepsilon(\vec{k})/K_B T} \sigma(\vec{x}, t) \right] d\vec{k} \\ &= \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta f|_{\Gamma_{N^+}} d\vec{k} + p \int_{\vec{v} \cdot \eta < 0} \vec{v} \cdot \eta f(\vec{x}, \vec{k}', t)|_{\Gamma_{N^+}} d\vec{k} + (1-p)\sigma C \int_{\vec{v} \cdot \eta < 0} \vec{v} \cdot \eta e^{\frac{-\varepsilon(\vec{k})}{K_B T}} d\vec{k} \\ &= \sigma(\vec{x}, t) - p\sigma(\vec{x}, t) + (1-p)\sigma(\vec{x}, t)(-1) \\ &= 0 \end{aligned} \tag{5.54}$$

However, for $p(\vec{k})$ a function of the crystal momentum the same choice of $\sigma(\vec{x}, t)$ and $C(x)$ as in the diffusive case does not necessarily guarantee that the zero flux condition will be satisfied at Neumann boundaries. Therefore, a new condition for C in order to satisfy this condition must be derived. We derive it below.

The general mixed reflection BC can be formulated as

$$f(\vec{x}, \vec{k}, t)|_- = p(\vec{k})f|_+(\vec{x}, \vec{k}', t) + (1-p(\vec{k}))C'\sigma'\{f|_+\}(\vec{x}, t)e^{-\varepsilon(\vec{k})/K_B T}, \quad (\vec{x}, \vec{k}) \in \Gamma_N^-$$

where $\sigma'\{f|_+\}(\vec{x}, t)$ and C' are the function and parameter such that the point-wise zero flux condition is satisfied at the Neumann boundaries:

$$\begin{aligned} 0 &= \eta(\vec{x}) \cdot J(\vec{x}, t) \\ &= \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta f|_{\Gamma_{N^+}} d\vec{k} + \int_{\vec{v} \cdot \eta < 0} \vec{v} \cdot \eta \left[p(\vec{k})f(\vec{x}, \vec{k}', t)|_{\Gamma_{N^+}} + (1-p(\vec{k}))C'e^{\frac{-\varepsilon(\vec{k})}{K_B T}} \sigma'(\vec{x}, t) \right] d\vec{k} \end{aligned}$$

Since

$$0 = \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta f|_{\Gamma_{N^+}} d\vec{k} + \int_{\vec{v} \cdot \eta < 0} \vec{v} \cdot \eta p(\vec{k}) f(\vec{x}, \vec{k}', t)|_{\Gamma_{N^+}} d\vec{k} - \sigma'(\vec{x}, t) C' \int_{\vec{v} \cdot \eta < 0} (1-p(\vec{k})) |\vec{v} \cdot \eta| e^{\frac{-\varepsilon(\vec{k})}{K_B T}} d\vec{k}$$

we conclude then that

$$\sigma'\{f|_+\}(\vec{x}, t) = \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta f|_+ d\vec{k} - \int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| p(\vec{k}) f(\vec{x}, \vec{k}', t)|_+ d\vec{k} \tag{5.55}$$

$$C' \{ \eta(\vec{x}) \} = \left(\int_{\vec{v} \cdot \eta < 0} (1 - p(\vec{k})) |\vec{v} \cdot \eta| e^{\frac{-\epsilon}{\vec{K}_B T_L}} d\vec{k} \right)^{-1} \quad (5.56)$$

The general mixed reflection BC then has the specific form:

$$\begin{aligned} f(\vec{x}, \vec{k}, t)|_- &= p(\vec{k}) f|_+(\vec{x}, \vec{k}', t) \\ &+ (1 - p(\vec{k})) e^{-\frac{\epsilon(\vec{k})}{\vec{K}_B T}} \frac{\left(\int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta f|_+ d\vec{k} - \int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| p(\vec{k}) f(\vec{x}, \vec{k}', t)|_+ d\vec{k} \right)}{\int_{\vec{v} \cdot \eta < 0} (1 - p(\vec{k})) |\vec{v} \cdot \eta| e^{\frac{-\epsilon(\vec{k})}{\vec{K}_B T_L}} d\vec{k}}, \end{aligned}$$

with $(\vec{x}, \vec{k}) \in \Gamma_N^-, (\vec{x}, \vec{k}') \in \Gamma_N^+$ s.t. $\vec{v}(\vec{k}') = \vec{v}(\vec{k}) - 2(\vec{v}(\vec{k}) \cdot \eta)\eta$.

Notice that the product $C' \sigma'(\vec{x}, t)$ has the form:

$$C' \sigma'(\vec{x}, t) = \frac{\left(\int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta f|_+ d\vec{k} - \int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| p(\vec{k}) f(\vec{x}, \vec{k}', t)|_+ d\vec{k} \right)}{\int_{\vec{v} \cdot \eta < 0} (1 - p(\vec{k})) |\vec{v} \cdot \eta| e^{\frac{-\epsilon(\vec{k})}{\vec{K}_B T_L}} d\vec{k}} \quad (5.57)$$

which for the case of p constant, it reduces to the original function $\sigma(\vec{x}, t)$ and parameter $C \{ \eta(\vec{x}) \}$:

$$\begin{aligned} \text{If } p &= \text{ct}, \\ C' \sigma'(\vec{x}, t) &= \frac{\left(\int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta f|_+ d\vec{k} - p \int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| f(\vec{x}, \vec{k}', t)|_+ d\vec{k} \right)}{\int_{\vec{v} \cdot \eta < 0} (1 - p) |\vec{v} \cdot \eta| e^{\frac{-\epsilon(\vec{k})}{\vec{K}_B T_L}} d\vec{k}} \\ &= \frac{(1 - p) \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta f|_+ d\vec{k}}{(1 - p) \int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| e^{\frac{-\epsilon(\vec{k})}{\vec{K}_B T_L}} d\vec{k}} \\ &= \frac{\int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta f|_+ d\vec{k}}{\int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| e^{\frac{-\epsilon(\vec{k})}{\vec{K}_B T_L}} d\vec{k}} \\ &= C \sigma(\vec{x}, t). \end{aligned}$$

However, for the non-constant case $p(\vec{k})$ the new function and parameter $\sigma'(\vec{x}, t)$, $C'(\eta)$ need to be used instead, as the previous $\sigma(\vec{x}, t)$, $C(\eta)$ won't satisfy the zero flux condition in general for $p(\vec{k})$:

$$\begin{aligned} 0 &= \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta f|_+ d\vec{k} + \int_{\vec{v} \cdot \eta < 0} \vec{v} \cdot \eta p(\vec{k}) f(\vec{x}, \vec{k}', t)|_+ d\vec{k} - \sigma' C' \int_{\vec{v} \cdot \eta < 0} (1 - p(\vec{k})) |\vec{v} \cdot \eta| e^{\frac{-\epsilon}{\vec{K}_B T_L}} d\vec{k} \\ C' \sigma' &= \frac{\int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta f|_+ d\vec{k} + \int_{\vec{v} \cdot \eta < 0} \vec{v} \cdot \eta p(\vec{k}) f(\vec{x}, \vec{k}', t)|_+ d\vec{k}}{\int_{\vec{v} \cdot \eta < 0} (1 - p(\vec{k})) |\vec{v} \cdot \eta| e^{\frac{-\epsilon}{\vec{K}_B T_L}} d\vec{k}} \\ &\neq \frac{\int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta f|_+ d\vec{k}}{\int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| e^{\frac{-\epsilon(\vec{k})}{\vec{K}_B T_L}} d\vec{k}} = C \sigma(\vec{x}, t) \quad \text{in general for } p(\vec{k}). \end{aligned}$$

A more general possible case of mixed reflection BC would have a specular parameter $p(\vec{x}, \vec{k}, t)$ dependent on position, momentum, and time. The related reflective BC would then be

$$f|_-(\vec{x}, \vec{k}, t) = p(\vec{x}, \vec{k}, t)f|_+(\vec{x}, \vec{k}', t) + \left(1 - p(\vec{x}, \vec{k}, t)\right) C^*(\vec{x}, t)\sigma^*(\vec{x}, t)M(\vec{x}, \vec{k})$$

$$(\vec{x}, \vec{k}) \in \Gamma_{N-}, \quad \text{and} \quad (\vec{x}, \vec{k}') \in \Gamma_{N+}. \quad (5.58)$$

where $M(\vec{x}, \vec{k})$ is the distribution to which the electrons get into equilibrium when reflecting diffusively on the physical boundary. $\sigma^*(\vec{x}, t)$ and $C^*(\vec{x}, t)$ are the functions such that the zero flux condition is satisfied pointwise at insulating boundaries:

$$\begin{aligned} 0 &= \eta(\vec{x}) \cdot \int_{\Omega_{\vec{k}}} \vec{v}(\vec{k}) f d\vec{k} = \int_{\vec{v} \cdot \eta > 0} \eta(\vec{x}) \cdot \vec{v}(\vec{k}) f|_+ d\vec{k} + \int_{\vec{v} \cdot \eta < 0} \eta(\vec{x}) \cdot \vec{v}(\vec{k}) f|_- d\vec{k} \\ &= \int_{\vec{v} \cdot \eta > 0} \eta \cdot \vec{v} f|_+ d\vec{k} + \int_{\vec{v} \cdot \eta < 0} \eta \cdot \vec{v} \left[p(\vec{x}, \vec{k}, t) f|_+(\vec{x}, \vec{k}', t) + \left(1 - p(\vec{x}, \vec{k}, t)\right) C^*(\vec{x}, t)\sigma^*(\vec{x}, t)M(\vec{x}, \vec{k}) \right] d\vec{k} \\ &= \int_{\vec{v} \cdot \eta > 0} \eta \cdot \vec{v} f|_+ d\vec{k} + \int_{\vec{v} \cdot \eta < 0} \eta \cdot \vec{v} p(\vec{x}, \vec{k}, t) f|_+(\vec{x}, \vec{k}', t) d\vec{k} \\ &\quad - \sigma^*(\vec{x}, t) C^*(\vec{x}, t) \int_{\vec{v} \cdot \eta < 0} |\eta \cdot \vec{v}| \left(1 - p(\vec{x}, \vec{k}, t)\right) M(\vec{x}, \vec{k}) d\vec{k} \end{aligned}$$

Therefore we conclude for this reflection case that

$$\sigma^*\{f|_+\}(\vec{x}, t) = \int_{\vec{v} \cdot \eta > 0} |\eta \cdot \vec{v}| f|_+ d\vec{k} - \int_{\vec{v} \cdot \eta < 0} |\eta \cdot \vec{v}| p(\vec{x}, \vec{k}, t) f|_+(\vec{x}, \vec{k}', t) d\vec{k} \quad (5.59)$$

$$C^*(\vec{x}, t) = \left(\int_{\vec{v} \cdot \eta < 0} |\eta \cdot \vec{v}| \left(1 - p(\vec{x}, \vec{k}, t)\right) M(\vec{x}, \vec{k}) d\vec{k} \right)^{-1} \quad (5.60)$$

and then the full BC formula for the $p(\vec{x}, \vec{k}, t)$ reflection case is

$$f|_-(\vec{x}, \vec{k}, t) = p(\vec{x}, \vec{k}, t) f|_+(\vec{x}, \vec{k}', t) + \left(1 - p(\vec{x}, \vec{k}, t)\right) M(\vec{x}, \vec{k}) \frac{\left[\int_{\vec{v} \cdot \eta > 0} |\eta \cdot \vec{v}| f|_+ d\vec{k} - \int_{\vec{v} \cdot \eta < 0} |\eta \cdot \vec{v}| p(\vec{x}, \vec{k}, t) f|_+(\vec{x}, \vec{k}', t) d\vec{k} \right]}{\int_{\vec{v} \cdot \eta < 0} |\eta \cdot \vec{v}| \left(1 - p(\vec{x}, \vec{k}, t)\right) M(\vec{x}, \vec{k}) d\vec{k}}$$

5.3.1 Numerical Implementation

The numerical implementation of the general mixed reflection with specular parameter $p(\vec{k})$ is done in such a way that a numerical equivalent of the point-wise zero flux condition is achieved.

The general mixed reflection boundary condition in our DG numerical scheme is

$$\begin{aligned}
\Phi_h|_- &= \Pi_h \{F_M(\Phi_h|_+)\} \\
&= \Pi_h \{p(\vec{w})\Phi_h|_+(\vec{x}, \vec{w}', t) + (1 - p(\vec{w}))C'\sigma'_h\{\Phi_h|_+\}(\vec{x}, t)e^{-w}s(w)\}.
\end{aligned} \tag{5.61}$$

We will be using the notation

$$\vec{w} = (w, \mu, \varphi), \quad d\vec{w} = dw d\mu d\varphi, \quad \vec{w}' = (w, \mu, \pi - \varphi). \tag{5.62}$$

The specific form of C' and σ' will be deduced from the numerical analogous of the mixed reflection boundary condition. We want to satisfy numerically the zero flux condition

$$\begin{aligned}
0 &= \eta(\vec{x}) \cdot \int_{\Omega_{\vec{w}}} \vec{v}(\vec{w}) \Phi_h d\vec{w} \\
&= \int_{\vec{v} \cdot \eta > 0} \vec{v}(\vec{w}) \cdot \eta \Phi_h|_+ d\vec{w} + \int_{\vec{v} \cdot \eta < 0} \vec{v}(\vec{w}) \cdot \eta \Phi_h|_- d\vec{w} \\
&= \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta \Phi_h|_+ d\vec{w} + \int_{\vec{v} \cdot \eta < 0} \vec{v} \cdot \eta \Pi_h \{p(\vec{w})\Phi_h|_+(\vec{x}, \vec{w}', t) + (1 - p(\vec{w}))C'\sigma'_h(\vec{x}, t)e^{-w}s(w)\} d\vec{w} \\
&= \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta \Phi_h|_+ d\vec{w} - \int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| \Pi_h \{p(\vec{w})\Phi_h|_+(\vec{x}, \vec{w}', t)\} d\vec{w} \\
&+ \int_{\vec{v} \cdot \eta < 0} \vec{v} \cdot \eta \Pi_h \{(1 - p(\vec{w}))C'\sigma'_h(\vec{x}, t)e^{-w}s(w)\} d\vec{w}
\end{aligned} \tag{5.63}$$

In the space V_h of piecewise continuous polynomials which are tensor products of polynomials of degree p in \vec{x} and of degree q in \vec{w} , the following holds:

$$\begin{aligned}
\Pi_h \{f_1(\vec{x})f_2(\vec{w})\} &= \Pi_h \{f_1(\vec{x})\} \Pi_h \{f_2(\vec{w})\}, \\
V_h &= \{v : v|_{\Omega_{ijkmn}} \in Q^{p,q}(\Omega_{ijkmn}) = P^p(X_{ij}) \otimes P^q(K_{kmn})\}.
\end{aligned} \tag{5.65}$$

Therefore, we have for our particular case that

$$\Pi_h \{(1 - p(\vec{w}))C'\sigma'_h(\vec{x}, t)e^{-w}s(w)\} = C'\sigma'_h(\vec{x}, t) \left[\sum_{k,m,n} \chi_{kmn} \frac{\int_{K_{kmn}} (1 - p(\vec{w}))e^{-w}s(w) d\vec{w}}{\int_{K_{kmn}} d\vec{w}} \right]$$

Using this, our numerical pointwise zero flux condition is

$$\begin{aligned}
0 &= \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta \Phi_h|_+ d\vec{w} - \int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| \Pi_h \{p(\vec{w}) \Phi_h|_+(\vec{x}, \vec{w}', t)\} d\vec{w} \\
&+ \int_{\vec{v} \cdot \eta < 0} \vec{v} \cdot \eta C' \sigma'_h(\vec{x}, t) \left[\sum_{k,m,n} \chi_{kmn} \frac{\int_{K_{kmn}} (1-p(\vec{w})) e^{-w} s(w) d\vec{w}}{\int_{K_{kmn}} d\vec{w}} \right] d\vec{w} \\
&= \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta \Phi_h|_+ d\vec{w} - \int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| \Pi_h \{p(\vec{w}) \Phi_h|_+(\vec{x}, \vec{w}', t)\} d\vec{w} \\
&+ C' \sigma'_h(\vec{x}, t) \int_{\vec{v} \cdot \eta < 0} \vec{v} \cdot \eta \left[\sum_{k,m,n} \chi_{kmn} \frac{\int_{K_{kmn}} (1-p(\vec{w})) e^{-w} s(w) d\vec{w}}{\int_{K_{kmn}} d\vec{w}} \right] d\vec{w} \\
&= \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta \Phi_h|_+ d\vec{w} - \int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| \Pi_h \{p(\vec{w}) \Phi_h|_+(\vec{x}, \vec{w}', t)\} d\vec{w} \\
&- C' \sigma'_h(\vec{x}, t) \sum_{k,m,n} \chi_{kmn} \int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| d\vec{w} \frac{\int_{K_{kmn}} (1-p(\vec{w})) e^{-w} s(w) d\vec{w}}{\int_{K_{kmn}} d\vec{w}} \\
&= \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta \Phi_h|_+ d\vec{w} - \int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| \Pi_h \{p(\vec{w}) \Phi_h|_+(\vec{x}, \vec{w}', t)\} d\vec{w} \\
&- \sigma'_h(\vec{x}, t) C' \sum_{k,m,n, \vec{v} \cdot \eta < 0} \int_{K_{kmn}} |\vec{v} \cdot \eta| d\vec{w} \frac{\int_{K_{kmn}} (1-p(\vec{w})) e^{-w} s(w) d\vec{w}}{\int_{K_{kmn}} d\vec{w}}
\end{aligned}$$

We conclude then that we can achieve a numerical equivalent of the pointwise zero flux condition by defining

$$\sigma'_h \{ \Phi_h|_+ \}(\vec{x}, t) = \int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta \Phi_h|_+ d\vec{w} - \int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| \Pi_h \{p(\vec{w}) \Phi_h|_+(\vec{x}, \vec{w}', t)\} d\vec{w} \quad (5.66)$$

$$(C' \{ \eta \})^{-1} = \sum_{k,m,n, \vec{v} \cdot \eta < 0} \int_{K_{kmn}} |\vec{v} \cdot \eta| d\vec{w} \frac{\int_{K_{kmn}} (1-p(\vec{w})) e^{-w} s(w) d\vec{w}}{\Delta w_k \Delta \mu_m \Delta \varphi_n} \quad (5.67)$$

Therefore, the inflow BC in our DG numerical method is given by the expression

$$\begin{aligned}
\Phi_h|_- &= \Pi_h \{p(\vec{w}) \Phi_h|_+(\vec{x}, \vec{w}', t)\} \\
&+ \Pi_h \left\{ (1-p(\vec{w})) C' \left(\int_{\vec{v} \cdot \eta > 0} \vec{v} \cdot \eta \Phi_h|_+ d\vec{w} - \int_{\vec{v} \cdot \eta < 0} |\vec{v} \cdot \eta| \Pi_h \{p(\vec{w}) \Phi_h|_+(\vec{x}, \vec{w}', t)\} d\vec{w} \right) e^{-w} s(w) \right\}.
\end{aligned}$$

The particular form of the coefficients defining the piecewise polynomial approximation $\Phi_h|_-$ for the general mixed reflection BC is presented below for the boundary $y = L_y$, since the calculations for the case of the boundary $y = 0$ are analogous.

For the boundary $y_{N_y+1/2} = L_y$, $\eta \cdot \vec{v} \propto +\hat{y} \cdot \vec{g} = g_2 \propto \cos \varphi$, which defines the sign of g_2 . Outflow cells have the index $j = N_y$. They are cells inside the

domain adjacent to the boundary. Inflow cells have the index $j = N_y + 1$. They are ghost cells adjacent to the boundary. We have in our case that

$$\begin{aligned}\sigma'_h &= \int_{\cos \varphi > 0} g_2 \Phi_h|_+ d\vec{w} - \int_{\cos \varphi < 0} |g_2| \Pi_h \{p(\vec{w}) \Phi_h|_+(\vec{x}, \vec{w}', t)\} d\vec{w} \\ &= \sum_{\substack{n \leq N_\varphi/2 \\ k, m, n}} \int_{K_{kmn}} g_2 \Phi_h|_+ d\vec{w} - \sum_{\substack{n > N_\varphi/2 \\ k, m, n}} \int_{K_{kmn}} |g_2| \Pi_h \{p(\vec{w}) \Phi_h|_+(\vec{x}, \vec{w}', t)\} d\vec{w}\end{aligned}$$

If $I = (i, N_y + 1, k, m, n)$ (inflow), $I' = (i, N_y, k, m, n')$, $n' = N'_\varphi - n + 1$ (outflow), the projection integrand is given by

$$\Pi_h \{p(\vec{w}) \Phi_h|_+(\vec{x}, \vec{w}', t)\} = \sum_I^{n > N_\varphi/2} \chi_I \frac{\int_{kmn} p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}} \left[T_{I'} + X_{I'} \frac{(x - x_i)}{\Delta x_i/2} + Y_{I'} (+1) \right]$$

The coefficients of σ'_h are given below. We have now that $I = (i, N_y, k, m, n)$, $I' = (i, N_y, k, m, n')$, $n' = N'_\varphi - n + 1$, so from the previous two formulas then

$$\begin{aligned}\sigma_I^0 &= \sum_{\substack{n \leq N_p/2 \\ k, m, n}} T_I(t) \int_k \frac{\sqrt{w(1 + \alpha_K w)}}{1 + 2\alpha_K w} dw \int_m \sqrt{1 - \mu^2} d\mu \int_n \cos \varphi d\varphi \\ &\quad - \sum_{\substack{n > N_p/2 \\ k, m, n}} T_{I'}(t) \int_k \frac{\sqrt{w(1 + \alpha_K w)}}{1 + 2\alpha_K w} dw \int_m \sqrt{1 - \mu^2} d\mu \int_n \cos \varphi d\varphi \frac{\int_{kmn} p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}} \\ \sigma_I^x &= \sum_{\substack{n \leq N_p/2 \\ k, m, n}} X_I(t) \int_k \frac{\sqrt{w(1 + \alpha_K w)}}{1 + 2\alpha_K w} dw \int_m \sqrt{1 - \mu^2} d\mu \int_n \cos \varphi d\varphi \\ &\quad - \sum_{\substack{n > N_p/2 \\ k, m, n}} X_{I'}(t) \int_k \frac{\sqrt{w(1 + \alpha_K w)}}{1 + 2\alpha_K w} dw \int_m \sqrt{1 - \mu^2} d\mu \int_n \cos \varphi d\varphi \frac{\int_{kmn} p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}} \\ \sigma_I^y &= \sum_{\substack{n \leq N_p/2 \\ k, m, n}} Y_I(t) \int_k \frac{\sqrt{w(1 + \alpha_K w)}}{1 + 2\alpha_K w} dw \int_m \sqrt{1 - \mu^2} d\mu \int_n \cos \varphi d\varphi \\ &\quad - \sum_{\substack{n > N_p/2 \\ k, m, n}} Y_{I'}(t) \int_k \frac{\sqrt{w(1 + \alpha_K w)}}{1 + 2\alpha_K w} dw \int_m \sqrt{1 - \mu^2} d\mu \int_n \cos \varphi d\varphi \frac{\int_{kmn} p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}}.\end{aligned}\tag{5.68}$$

Since on one hand we have

$$\begin{aligned}\Phi_h|_{L_y}^- &= \Pi_h \{p(\vec{w}) \Phi_h|_+(\vec{x}, \vec{w}', t)\} + \Pi_h \{(1 - p(\vec{w})) C' \sigma'_h \{\Phi_h|_+\}(\vec{x}, t) e^{-w} s(w)\} \\ &= \sum_{\substack{n > N_\varphi/2 \\ i, k, m, n}} \chi_{i, N_y + 1, k, m, n} \frac{\int_{kmn} p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}} \left[T_{i, N_y, k, m, n'} + X_{i, N_y, k, m, n'} \frac{(x - x_i)}{\Delta x_i/2} + Y_{i, N_y, k, m, n'} \cdot 1 \right] \\ &\quad + \sum_{\substack{n > N_\varphi/2 \\ i, k, m, n}} \chi_{i, N_y + 1, k, m, n} \frac{\int_{kmn} (1 - p(\vec{w})) e^{-w} s(w) d\vec{w}}{\int_{kmn} d\vec{w}} \times \\ &\quad \times C' \left[\sigma_{i, N_y, k, m, n}^0 + \sigma_{i, N_y, k, m, n}^x \frac{(x - x_i)}{\Delta x_i/2} + \sigma_{i, N_y, k, m, n}^y (+1) \right]\end{aligned}$$

and on the other hand

$$\Phi_h|_{y_{N_y+1/2}}^- = \sum_{i,k,m,n} \chi_{i,N_y+1,k,m,n} \left[T_{i,N_y+1,k,m,n} + X_{i,N_y+1,k,m,n} \frac{(x-x_i)}{\Delta x_i/2} + Y_{i,N_y+1,k,m,n}(-1) \right]$$

we conclude that the coefficients for $\Phi_h|_-$ are then

$$\begin{aligned} T_{i,N_y+1,k,m,n} &= T_{I'} \frac{\int_{kmn} p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}} + C' \sigma_I'^0 \frac{\int_{kmn} (1-p(\vec{w})) e^{-w} s(w) d\vec{w}}{\int_{kmn} d\vec{w}}, \\ X_{i,N_y+1,k,m,n} &= X_{I'} \frac{\int_{kmn} p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}} + C' \sigma_I'^x \frac{\int_{kmn} (1-p(\vec{w})) e^{-w} s(w) d\vec{w}}{\int_{kmn} d\vec{w}}, \\ Y_{i,N_y+1,k,m,n} &= - \left(Y_{I'} \frac{\int_{kmn} p(\vec{w}) d\vec{w}}{\int_{kmn} d\vec{w}} + C' \sigma_I'^y \frac{\int_{kmn} (1-p(\vec{w})) e^{-w} s(w) d\vec{w}}{\int_{kmn} d\vec{w}} \right), \\ I' &= (i, N_y, k, m, n'), \quad I = (i, N_y, k, m, n). \end{aligned} \quad (5.69)$$

6 Preliminary Numerical Results

We present results of preliminary numerical simulations for the case of a 2D n bulk silicon diode with an applied bias between the boundaries $x = 0, L_x$, and reflection BC at the boundaries $y = 0, L_y$. The required dimensionality in momentum space is 3D $\vec{k}(w, \mu, \varphi)$. The specifics of our simulations are:

Initial Condition: $\Phi(w)|_{t=0} = \Pi \{N e^{-w} s(w)\}$. Final Time: 1.0ps

Boundary Conditions (BC):

\vec{k} -space: Cut-off - at $w = w_{max}$, Φ is machine zero.

Only needed BC in (w, μ, φ) : transport normal to the boundary analitically zero at 'singular points' boundaries:

At $w = 0, g_3 = 0$. At $\mu = \pm 1, g_4 = 0$. At $\varphi = 0, \pi, g_5 = 0$.

\vec{x} -space: Charge Neutrality at boundaries $x = 0, x = 0.15\mu m$.

Bias - Potential: $V|_{x=0} = 0.5235$ V, $V|_{x=0.15\mu m} = 1.5235$ V.

Neumann BC for Potential at $y = 0, L_y = 12nm$: $\partial_y V|_{y=0, L_y} = 0$.

Reflection BC at $y = 0, y = 12nm$: Specular, Diffusive, & Mixed with $p = 0.5$.

We observe an influence of the Diffusive and Mixed Reflection in macroscopic observables, particularly noticeable in the kinetic moments. For example, the distribution of charges slightly increases with diffusive reflection close to reflecting boundaries, and alters the density profile over domain, due to mass conservation. Momentum & Velocity increase with diffusive reflection over the domain, while the energy is decreased by Diffusive Reflection over the domain.

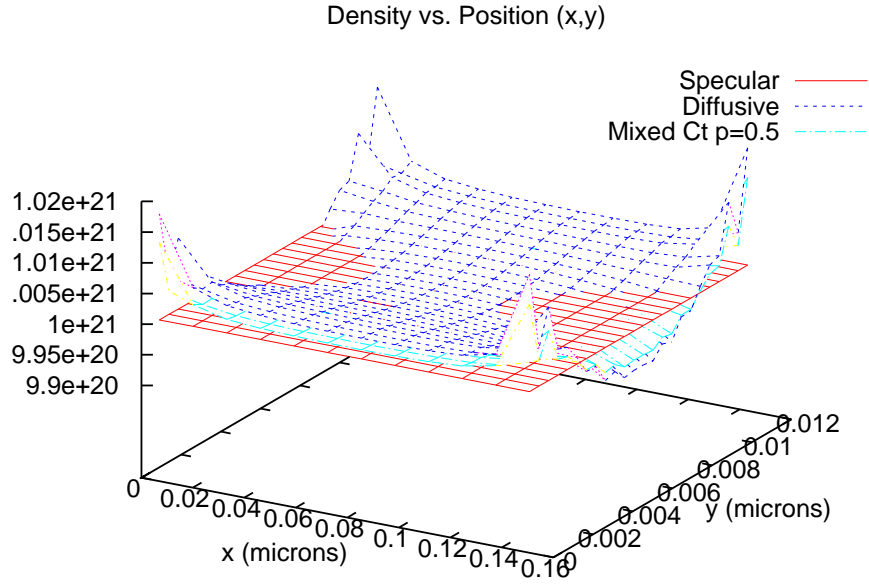


Figure 6.2: Density ρ (m^{-3}) vs Position (x,y) in (μm) plot for Specular, Diffusive, & Mixed $p = 0.5$ Reflection.

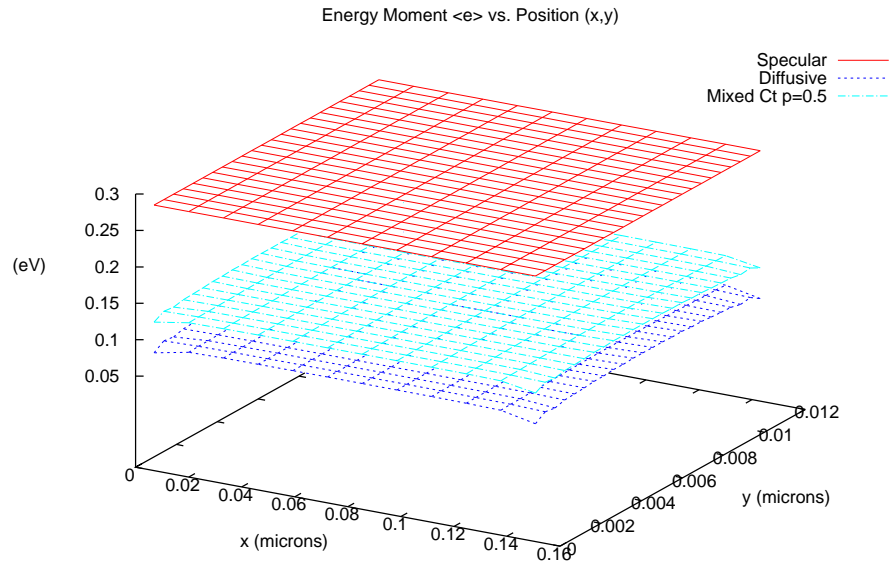


Figure 6.3: Mean energy e (eV) vs. Position (x,y) in (μm) plots for Specular, Diffusive, & Mixed $p = 0.5$ Reflection.

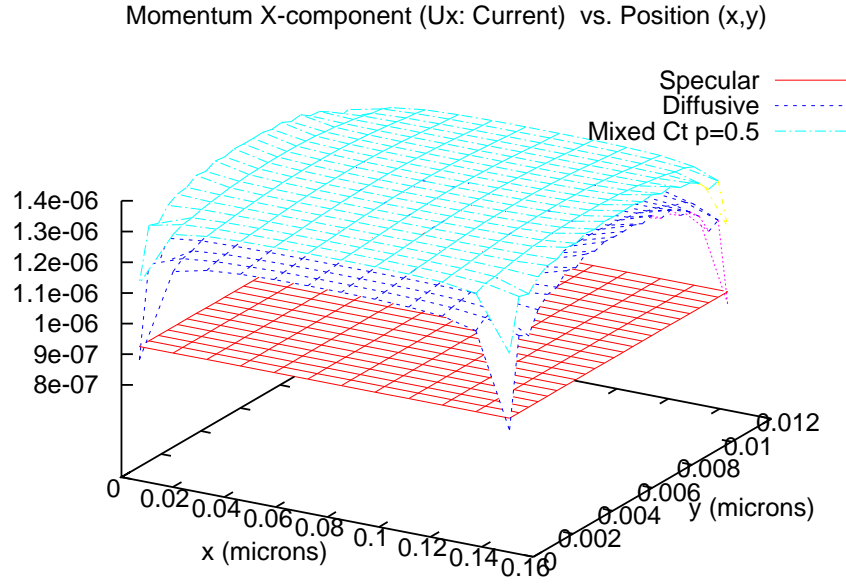


Figure 6.4: Momentum U_x ($10^{28} \frac{cm^{-2}}{s}$) vs. Position (x, y) in (μm) for Specular, Diffusive, and Mixed $p = 0.5$ Reflection.

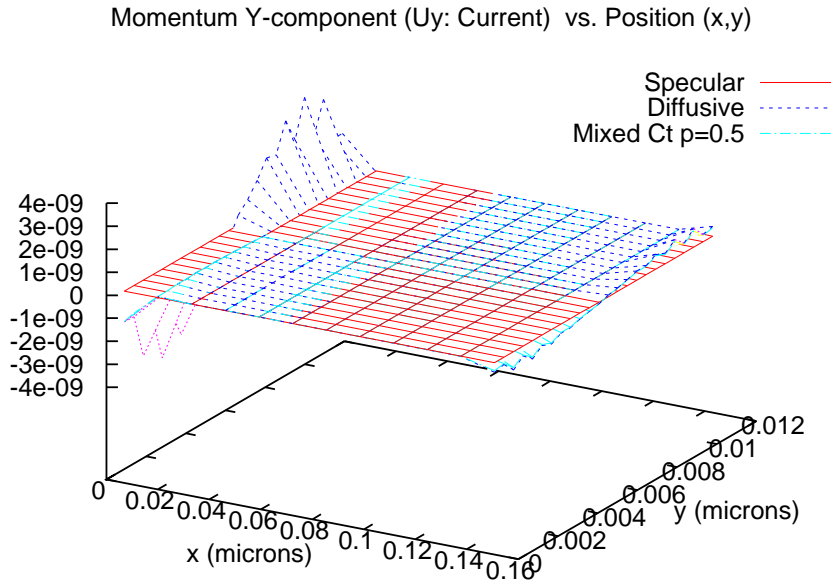


Figure 6.5: Momentum U_y ($10^{28} \frac{cm^{-2}}{s}$) vs. Position (x, y) in (μm) for Specular, Diffusive, and Mixed $p = 0.5$ Reflection.

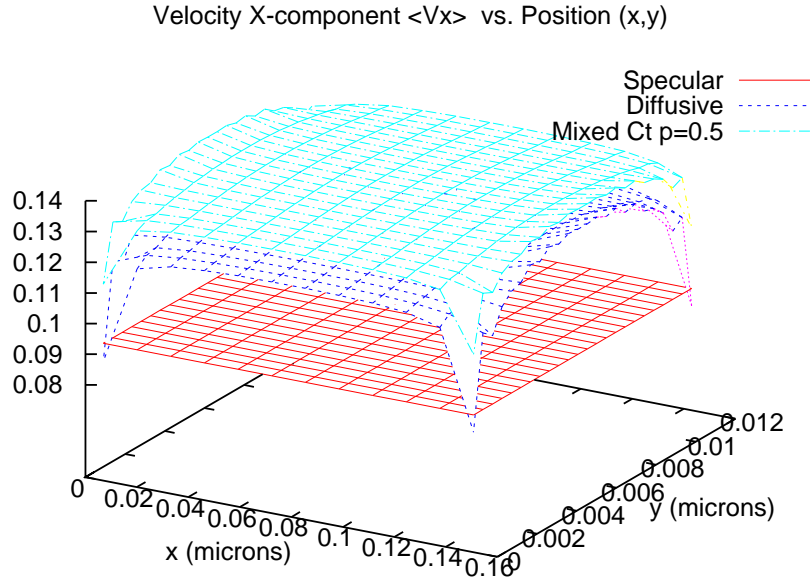


Figure 6.6: Mean Velocity V_x vs. Position (x, y) in (μm) for Specular, Diffusive, and Mixed $p = 0.5$ Reflection.

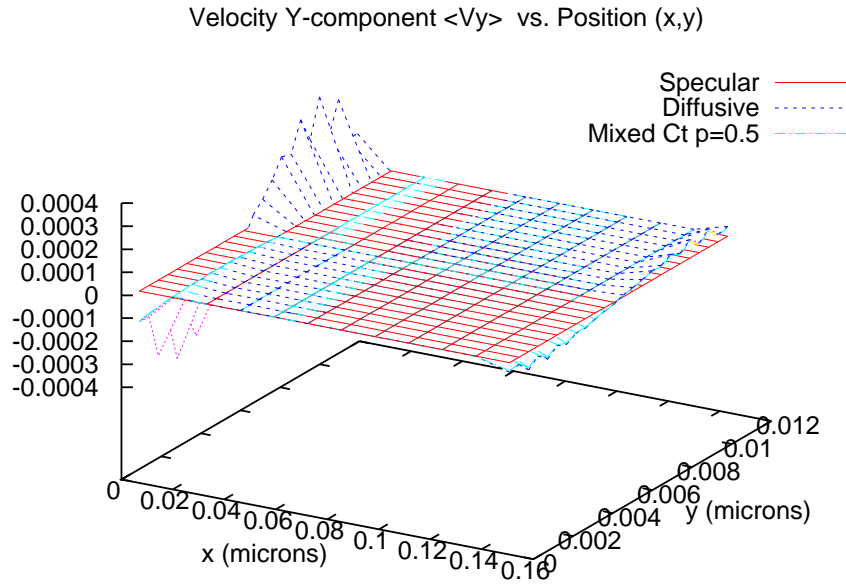


Figure 6.7: Mean Velocity V_y vs. Position (x, y) in (μm) for Specular, Diffusive, and Mixed $p = 0.5$ Reflection.

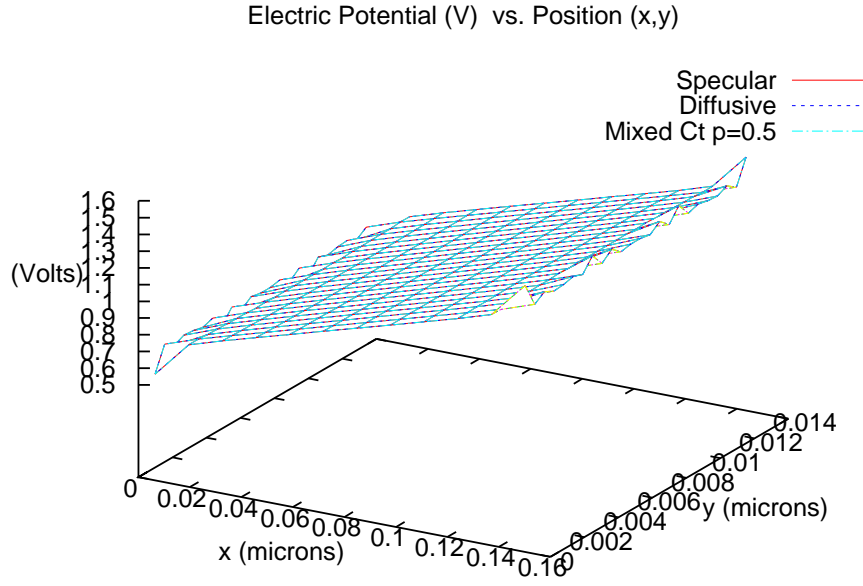


Figure 6.8: Potential $V(Volts)$ vs. Position (x,y) (μm) plot for Specular, Diffusive & Mixed $p = 0.5$ Reflection

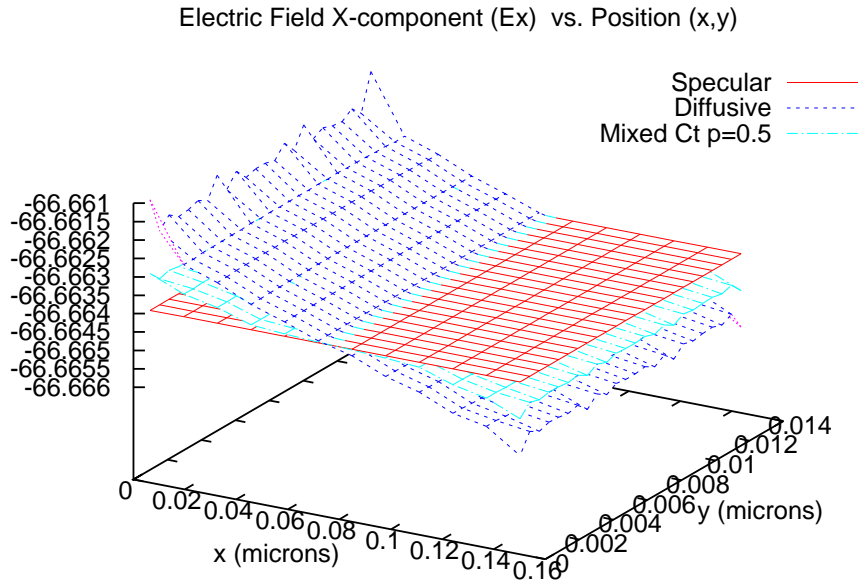


Figure 6.9: Electric Field Component E_x vs. Position (x,y) in (μm) for Specular, Diffusive & Mixed $p = 0.5$ Reflection

7 Conclusions

We have considered the mathematical and numerical modeling of Reflective Boundary Conditions in 2D devices and their implementation in DG-BP schemes. We have studied the specular, diffusive and mixed reflection BC on physical boundaries of the device for the modeling of surface roughness, comparing the influence of these different reflection cases in the computational prediction of moments close to the boundaries and their associated scale.

There is an effect due to diffusive reflection at Neumann boundaries over the moments of the probability density function, whose influence is not only restricted to the boundaries but actually to the whole domain, partly due to mass conservation.

Work in progress is being developed for the computational implementation for Mixed Reflection with a $p(\vec{w})$, and the study of Reflective BC in a 2D double gate MOSFET device. Future Research will be related to Reflective BC with an EPM-DG-BP Full Band Model, and the inclusion of additional scattering mechanisms.

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